VISUALISING STATISTICAL MECHANICS. THE CASE OF ENERGY DISTRIBUTION

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1 INTRODUCTION

The main goal of statistical mechanics is to relate macroscopic properties of matter to microscopic characteristics of its constituent particles. Because of the large number of interacting particles usually involved in real macroscopic systems, statistical mechanics has to face several mathematical difficulties. This very often leads to the impossibility of performing the exact calculation of the thermodynamic properties, especially at undergraduate or high school level.

Today, some simulation tools designed to look at and visualise the behaviour of interacting micro-agents and patterns emerging from their interactions are available. Their use makes possible to obtain good estimations of thermodynamic properties of small systems of distinguishable/indistinguishable particles, when appropriate numerical computational procedures are applied.

In the following we deal with a pedagogical approach to simulate the behaviour of systems of classical/quantum non interacting identical particles constituting the classical/quantum ideal gas. In particular, we use the NetLogo modelling environment (http://ccl.northwestern.edu/netlogo/) to study some properties of ideal quantum Bose and Fermi gases; we obtain the Bose-Einstein (BE) and Fermi-Dirac (FD) distribution functions and compare these with the Maxwell-Boltzmann (MB) statistics. The main point of the approach is the application of the same evolution mechanisms to both classical and quantum particles that are, however, differentiated on the basis of their properties (distinguishability/indistinguishability, satisfying/not satisfying the Pauli principle).

2 THE METHOD

Instead of following the standard procedures elicited in statistical mechanics textbooks, where the knowledge of the system partition function leads, after some more or less complex calculations and approximations, to the distribution function and to the evaluation of the thermal properties, we will use an approach concerning a stochastic evolution of system microstates in state space. To achieve this aim, we assume that a generic system obeys a very simplified dynamics, such as a Markov chain [1] on a finite state space, satisfying the condition of detailed balance [1]. In particular, we assume that each particle can perform, at different

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time steps, a random walk within the single particle state space. The transition probabilities from one single particle state into another are opportunely chosen, for each particle type, according to the main characteristic of a Markov process of being a no-memory process (the statistical properties of the immediate future state are uniquely determined by the present one regardless of any other past states). In order to reach a steady state, the transition probabilities have also to fulfil the detailed balance condition. This, essentially, drives the system toward thermodynamic equilibrium by forcing direct and reverse transition probabilities between a given couples of state to be equal.

This way of modelling the system dynamics provides a good starting point in the development of a variant of the well known Metropolis algorithm [2], able to take into account for the effect of indistinguishability in simulating the behaviour of different systems of identical quantum particles.

The evolution of a system from a generic state to another can be reduced to a series of transitions of its constituent particles between all possible single particle states. This method of modelling the dynamics of the systems is especially useful to determine the average occupation number of single particle states. For transitions between two generic states i and j of energy ε_i and ε_j , respectively, the detailed balance condition takes the following form

$$\overline{n}_i \cdot T_{ij} = \overline{n}_j \cdot T_{ji} \ , \quad \forall i, j \ , \tag{1}$$

where $\overline{n}_i$ and $\overline{n}_j$ represent the average occupation number of the *i-th* and *j-th* single particle state while and T_{ij} and T_{ji} represent the transition probabilities from state i to state j, and vice versa, respectively.

For a system of distinguishable particles, statistical mechanics assumes, in agreement with theory and experiments, that at thermal equilibrium the average occupation number, $\overline{n}$, of a single particle state of energy ε is given by

$$\overline{n}(\varepsilon) = z \cdot e^{-\varepsilon / k_B T} \ , \tag{2}$$

where T is the absolute temperature, k_B is the Boltzmann constant and z = $\exp(\mu/k_BT)$ is a normalization factor, usually called fugacity that depends from the chemical potential, μ, and from T. By substituting eq. (2) in eq. (1) it is possible to find that a Markov chain, with transition probabilities given by the following ratio

$$\frac{T_{ij}}{T_{ji}} = \frac{\overline{n}(\varepsilon_j)}{\overline{n}(\varepsilon_i)} = \frac{z \cdot e^{-\varepsilon_j / k_B T}}{z \cdot e^{-\varepsilon_i / k_B T}} = \frac{e^{-\varepsilon_j / k_B T}}{e^{-\varepsilon_i / k_B T}} \ , \quad \forall i, j \tag{3}$$

asymptotically converges to the Maxwell-Boltzmann distribution.

The transition probabilities from a state i to a state j, T_{ij} , can be written as the product of the step probability, S_{ij} , to actually perform the transition times the probability, A_{ij} , to accept this transition, so that $T_{ij} = S_{ij} \cdot A_{ij}$.

For identical distinguishable particles, there are no restrictions on possible configurations of the particles, so probabilities S_{ij} may be chosen in order to fulfil a condition of symmetry, $S_{ij} = S_{ji}$, or even all equal. In both cases they cancel each other in (3), that is reduced to the following condition on the acceptance probabilities

$$\frac{A_{ij}}{A_{ji}} = \frac{e^{-\varepsilon_j / k_B T}}{e^{-\varepsilon_i / k_B T}}, \quad \forall i, j \ . \tag{4}$$

3 SIMULATIVE DEDUCTIONS OF PROBABILITY DISTRIBUTIONS

The simulation analysis of identical, non-interacting particles has been performed by using a Monte Carlo procedure, based on the Metropolis method that follows the dynamics of particles in the space of moments; i.e. we assume that particles are moving from a single particle state to another, where each state is characterized by a particular value of the moment, $\hbar\mathbf{k}$.

The typical Monte Carlo simulations of thermodynamic systems allow the system to evolve from one state to another so that, at the equilibrium, the state distribution is correctly described by the Boltzmann factors. The method consists in starting from an arbitrary initial state and in applying an algorithm to simulate the time evolution. For systems of distinguishable particles it is possible to choose S_{ij} = S_{ji} . So, to obtain the Boltzmann distribution it is sufficient to use the detailed balance (4) involving only the acceptance probability, A_{ij} . By assuming an arbitrary initial condition, a new state is chosen for each particles; then, the energy variation of the system is calculated ($\Delta E = E_{\text{new}} - E_{\text{old}}$) and if $\Delta E \leq 0$ the new state is accepted, otherwise it is accepted with probability $w = \exp(-\Delta E/k_B T)$. This condition can be implemented by comparing w with a random number r, uniformly distributed between 0 and 1 and accepting the new state if $w > r$.

From a physical point of view, the described choice of the acceptance probabilities drives the system to a minimum energy state. In fact, the configurations reducing the energy of the system are always accepted, while those increasing it are accepted with a probability proportional to the Boltzmann weight. By making the system evolve from one configuration to another it is possible to calculate various physical quantities of interest averaged on different system configurations, where a configuration is simply a list of how many particles occupy every single particle state. Different thermodynamic properties can be calculated, such as the distribution function, $\overline{n}(\varepsilon)$, the mean particle energy, $\langle E\rangle/N$, and the specific heat for particle, $c_V = (\langle E^2\rangle - \langle E\rangle^2)/Nk_B T^2$ obtained from energy fluctuations.

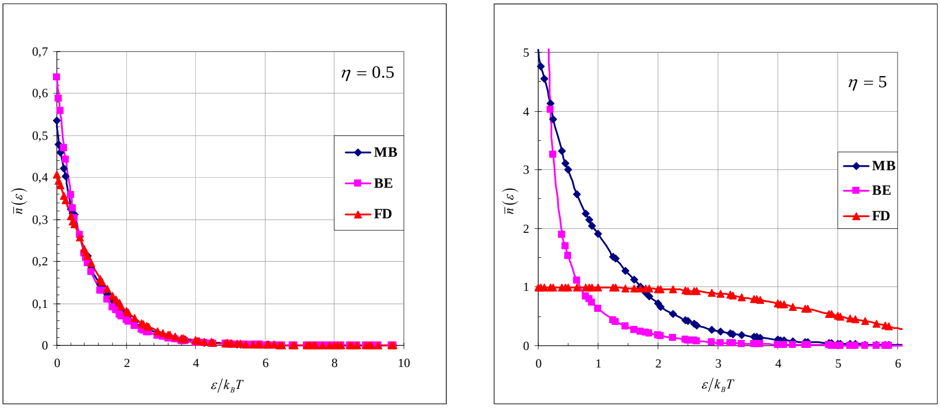
The procedure just discussed is very used in simulation of MB systems. In order to simulate systems of quantum particles, it was necessary to implement an algorithm able to take into account for indistinguishability; i.e., it was necessary to implement an algorithm able to reproduce the correct step probabilities $S_{ij} = (1 - \overline{n}_j)$ and $S_{ji} = (1 - \overline{n}_i)$ when they depend on the final state occupation, as it is in the case of systems of identical indistinguishable particles.

4 SIMULATION RESULTS

The simulations built on the basis of the described model can be used by students at a "user level", without entering into the algorithm coding the simulation itself and only explaining the fundamental rules used to represent the three different kinds of particles.

Simulations have been performed on a bi-dimensional (2D) systems consisting of 500 particles. This reduces computational time in calculating energy distributions and shows the possibility of a Bose condensation in spatial dimensions lower than three [3]. The three types of systems (such as FD, BE and MB) have been simulated with respect to the gas degeneracy parameter, η (in the 2D case $\eta \propto 1/T$). In Figure 1 a comparison between distribution functions, for two different values of η is reported. These distributions quite well agree with theoretical expectations for the same values of η [4].

In low degeneracy conditions (η = 0.5), the three distributions differ very little. On the other hand, increasing η (η = 5) the three distribution appear to be markedly different.



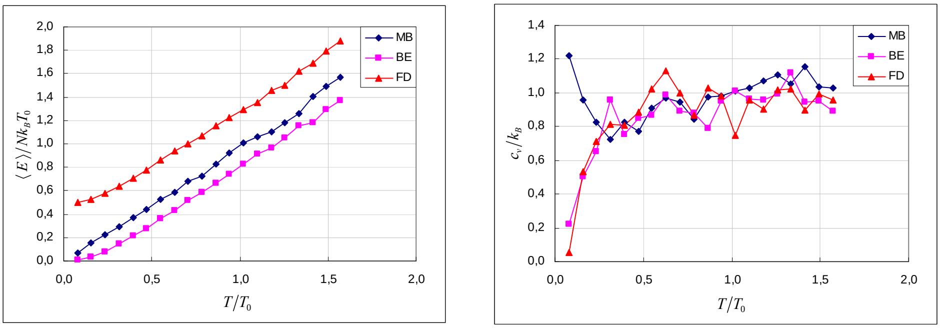
(a) (b)

Figure 1 Comparison between distribution functions for a 2D system. (a) Low degeneracy (η = 0.5); (b) high degeneracy (η = 5).

Increasing degeneracy the bosons tend to crowd the states of lowest energy, the fermions tend to fill in all the states of energy lower than the Fermi energy, while the MB distribution only changes for a scale factor. Figure 2 shows the simulation results with respect to the mean energy and specific heat as a function of temperature, for the three different systems of particles. The comparison between the graphs of particle mean energy shows that, while in MB the energy has a linear trend for all temperatures, in BE and FD for high temperatures it has the same trend than in MB, but tends to saturate when the temperature tends to zero. These results reflect in the trends of the particle specific heat. In fact, while in MB the specific heat fluctuates around a constant value irrespective of temperature, in BE and FD for high temperatures it has the same trend than in MB, but tends to zero as the temperature tends to zero.

Further information on the thermodynamic properties of the simulated systems, in particular on the trends of the chemical potential, $\mu = k_B T \ln z$ as a function of temperature, were obtained through an estimate of the mean occupation number of the ground state.

Figure 3 reports the trends of μ as a function of temperature for the three different 2D systems. It shows that in BE when T goes to zero μ goes also to zero, staying negative, while it becomes positive in FD. MB exhibit an intermediate trend for all temperatures and a maximum is present. This maximum takes into account the intermediate behaviour of MB particles with respect to FD and BE ones. In fact, when T goes to zero, MB particles tend to be more "unsocial" than BE and more "social" than FD particles. However, unlike fermions, nothing forbids them to condensate in the ground state when the temperature is zero. In bosons, however, this condensation occurs at a non-zero temperature. This condition is in accord to the fact that the system exhibits a Bose condensation.



(a) (b)

Figure 2 (a) Comparison between particle mean energy in the three different MB, BE and FD cases. (b) Comparison between particle specific heat in the three different MB, BE and FD cases.

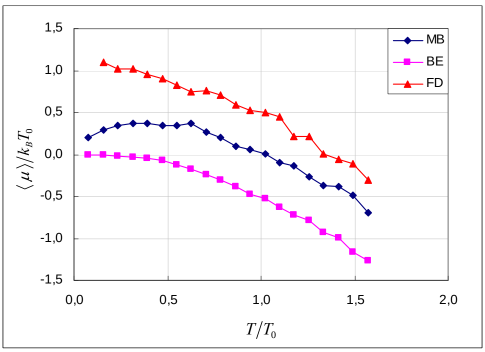


Figure 3 Comparison between chemical potential for the three type of systems.

5 CONCLUSIONS

We described an approach to simulate the behaviour of systems of classical/quantum non interacting identical particles representing classical/quantum ideal gasses. This approach was thought in order to simplify the introduction of these topics to undergraduate pupils without diverting them too much from the physical situation due to the mathematical difficulties related to the traditional statistical mechanics approach. The simulations were built by using the Net Logo simulation environment and tested in the framework of the Postgraduate School for Pre-Service Physics Teacher Education at University of Palermo. Preliminary results of tests reveal that trainee teachers have liked the easier approach to quantum distribution functions provided by the simple application of the detailed balance and the possibility to bypass the mathematical load of the classical approach to statistical mechanics.

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